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Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: MARK BERCH Examiner #: 59193 Date: 9 MAY 2005  
Art Unit: 1624 Phone Number: 2- 0663 Serial Number: 10608657  
Location (Bldg/Room#): 5C01 (Mailbox #): 5C18 Results Format Preferred (circle): PAPER DISK  
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To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following: my

Title of Invention: \_\_\_\_\_

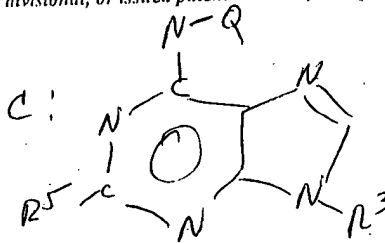
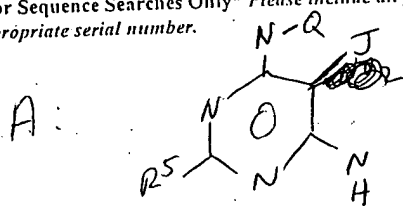
Inventors (please provide full names): \_\_\_\_\_

Earliest Priority Date: \_\_\_\_\_

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.



R5 = anything except OH

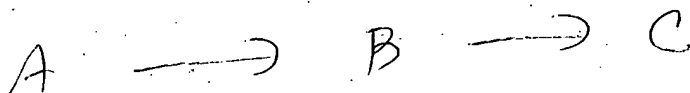
A: J = NO<sub>2</sub>

B: J = NH<sub>2</sub>

R3 = anything except Heterocycle

Q = Cl/Si

CASREACT



STAFF USE ONLY

Searcher: \_\_\_\_\_

Searcher Phone #: \_\_\_\_\_

Searcher Location: \_\_\_\_\_

Date Searcher Picked Up: \_\_\_\_\_

Date Completed: 5/12

Type of Search

\_\_\_\_ NA Sequence (#)

\_\_\_\_ AA Sequence (#)

5 Structure (#)

\_\_\_\_ Bibliographic

\_\_\_\_ Litigation

Vendors and cost where applicable

767.9 STN \_\_\_\_\_ Dialog

\_\_\_\_ Questel/Orbit \_\_\_\_\_ Lexis/Nexis

\_\_\_\_ Westlaw \_\_\_\_\_ WWW/Internet

\_\_\_\_ In-house sequence systems

\_\_\_\_ Commercial \_\_\_\_\_ Oligomer \_\_\_\_\_ Score/Length  
\_\_\_\_ Interference \_\_\_\_\_ SPDI \_\_\_\_\_ Encode/Transl

Searcher Prep+ Review Time 10

Online Time 10

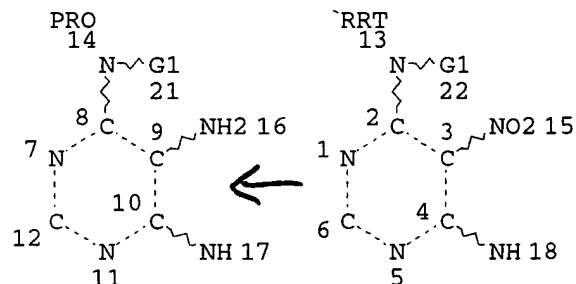
=&gt; d que 13

L1

STR

C @19

Si @20



VAR G1=19/20

NODE ATTRIBUTES:

NSPEC IS RC AT 19

NSPEC IS RC AT 20

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L3 5 SEA FILE=CASREACT SSS FUL L1 ( 6 REACTIONS)

=&gt; d 13 ibib abs crd 1-5

L3 ANSWER 1 OF 5 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 141:157094 CASREACT

TITLE: A new 2-carbamoyl pteridine that inhibits mycobacterial FtsZ

AUTHOR(S): Reynolds, R. C.; Srivastava, S.; Ross, L. J.; Suling, W. J.; White, E. L.

CORPORATE SOURCE: Drug Discovery Division, Southern Research Institute, Birmingham, AL, 35205, USA

SOURCE: Bioorganic &amp; Medicinal Chemistry Letters (2004), 14(12), 3161-3164

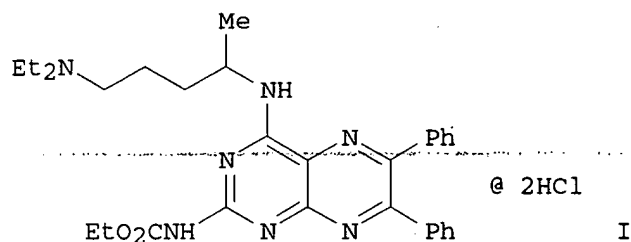
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

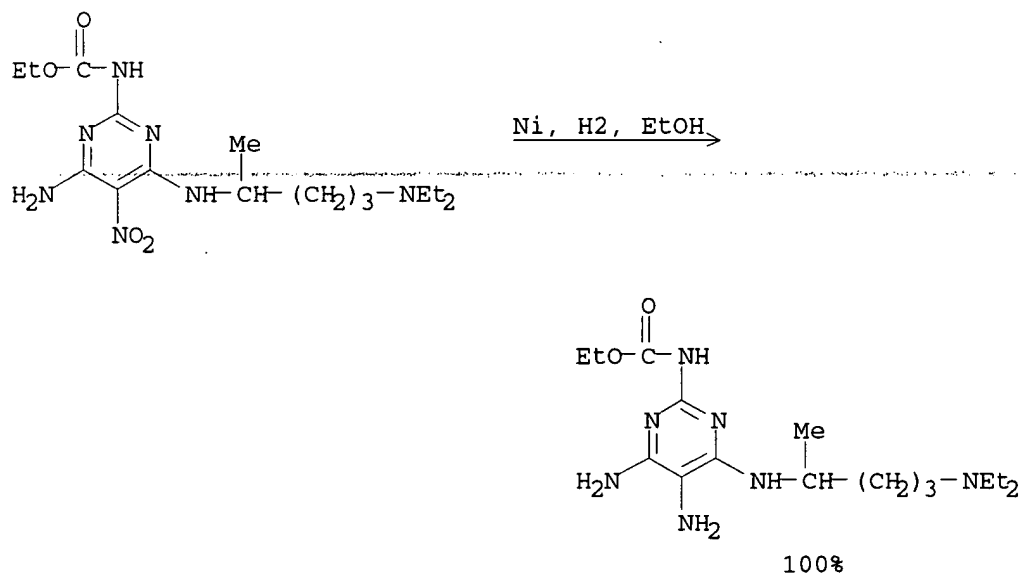
LANGUAGE: English

GI



AB The preparation of a new 2-carbamoyl pteridine (I), its activity data against FtsZ from *M. tuberculosis* (Mtb), and in vitro antibacterial data against Mtb strain H37Ra are presented.

RX(7) OF 28



NOTE: Raney nickel used

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 5 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 135:272791 CASREACT

TITLE: Synthesis of Bicyclic Pyrimidine Derivatives as ATP Analogues

AUTHOR(S): Makara, Gergely M.; Ewing, William; Ma, Yao; Wintner, Edward

CORPORATE SOURCE: NeoGenesis Drug Discovery, Cambridge, MA, 02139, USA

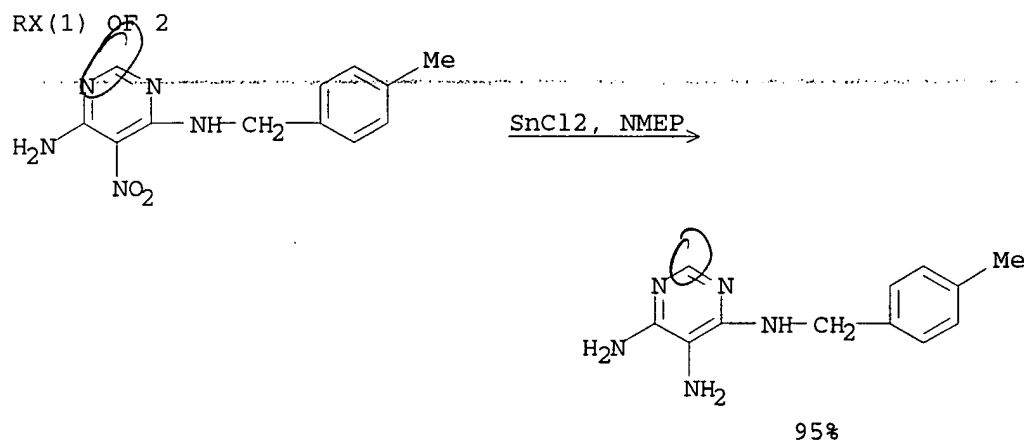
SOURCE: Journal of Organic Chemistry (2001), 66(17), 5783-5789  
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A highly efficient and general solid-phase synthesis of bicyclic pyrimidine derivs. that target purine dependent proteins is reported. The synthesis of the key intermediate, 4,6-disubstituted-5-amino-pyrimidine, involved reduction of the corresponding nitro derivs. using 1,1'-dioctyl-viologen in a triphasic milieu. The mild reduction conditions enable the use of any acid labile solid support as well as a wide range of combinatorial substituents, thus enabling the synthesis of large libraries of highly diverse bicyclic pyrimidines. Alternative reduction conditions with tin(II) chloride and structure-reactivity studies are discussed as well.



NOTE: solid-supported reaction

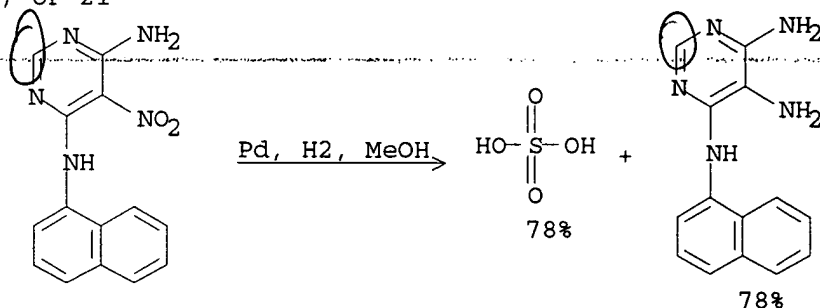
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 5 CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 113:58784 CASREACT  
 TITLE: Purine derivatives as competitive inhibitors of human erythrocyte membrane phosphatidylinositol 4-kinase  
 AUTHOR(S): Young, Rodney C.; Jones, Martin; Milliner, Kevin J.; Rana, Kishore K.; Ward, John G.  
 CORPORATE SOURCE: Smith Kline and French Res. Ltd., Welwyn/Hertfordshire, AL6 9AR, UK  
 SOURCE: Journal of Medicinal Chemistry (1990), 33(8), 2073-80 CODEN: JMCMAR; ISSN: 0022-2623  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

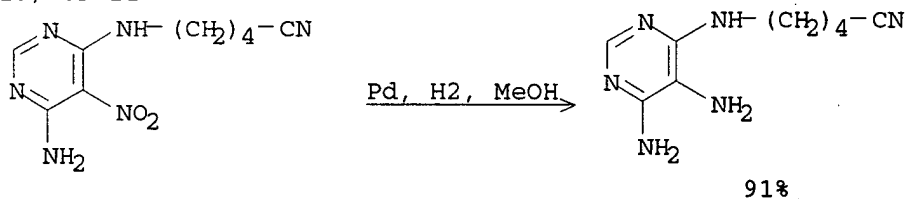
AB The possibility of deriving a potent, cell-penetrating inhibitor of human erythrocyte phosphatidylinositol 4-kinase, competitive with respect to ATP, has been investigated in a series of purine derivs. and analogs. The purine nucleus is not essential for binding to the ATP site but offers the advantage of synthetic accessibility to its derivs. The optimum substitution pattern in purine consisted of an electron-releasing substituent in the 6-position (e.g. amino, as in adenine) and a compact, lipophilic group in either the 8-position or, preferably, the 9-position, suggesting the importance of the N-1 lone pair and hydrophobic contributions of the 8- and 9-substituents to binding. The most potent

inhibitor synthesized was 9-cyclohexyladenine, which has an apparent  $K_i$  value of 3.7  $\mu\text{M}$ .

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RX(13) OF 21



L3 ANSWER 4 OF 5 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 112:35543 CASREACT

TITLE: Benzodiazepine receptor binding activity of 8-substituted-9-(3-substituted-benzyl)-6-(dimethylamino)-9H-purines

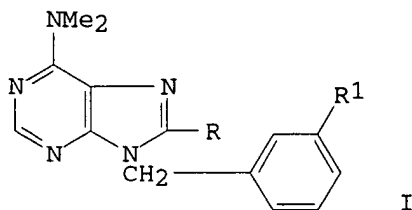
AUTHOR(S): Kelley, James L.; McLean, Ed W.; Linn, James A.; Krochmal, Mark P.; Ferris, Robert M.; Howard, James L.  
CORPORATE SOURCE: Div. Org. Chem., Burroughs Wellcome Co., Research Triangle Park, NC, 27709, USA

SOURCE: Journal of Medicinal Chemistry (1990), 33(1), 196-202  
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

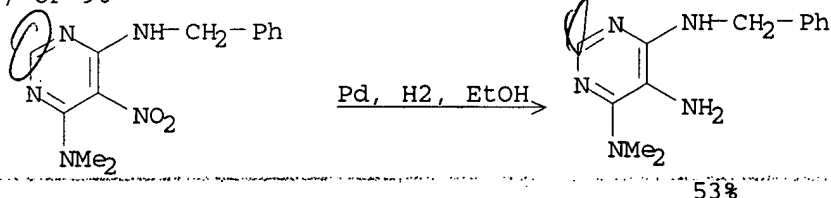
LANGUAGE: English

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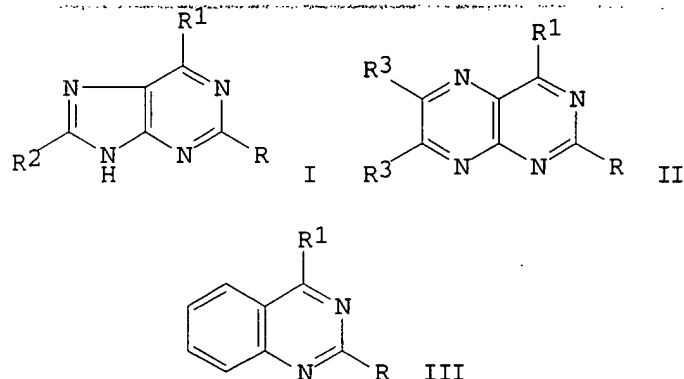


AB A series of 8-substituted analogs of 9-(3-aminobenzyl)-6-(dimethylamino)-9H-purine (I, R = H, R1 = NH2) were synthesized and tested for their ability to bind to the benzodiazepine receptor in rat brain tissue. The most active compound was I (R = Br, R1 = NHCHO) (ED50 = 0.011  $\mu$ M), which was 1000-fold more active than I (R = R1 = H) and nearly as active as diazepam. However, neither I (R = Br, R1 = NHCHO) nor 11 analogs exhibited significant anxiolytic activity on a modified Geller-Seifter Conflict schedule.

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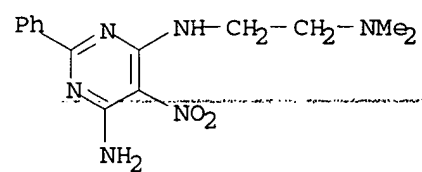
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 106:84257 CASREACT  
 TITLE: Heterocyclic amplifiers of phleomycin. VI. Some phenylpurines, phenylpteridines, phenylquinazolines and related compounds  
 AUTHOR(S): Brown, Desmond J.; Mori, Kenya  
 CORPORATE SOURCE: John Curtin Sch. Med. Res., Aust. Natl. Univ., Canberra, 2601, Australia  
 SOURCE: Australian Journal of Chemistry (1985), 38(3), 467-74  
 CODEN: AJCHAS; ISSN: 0004-9425  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



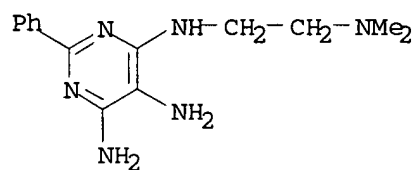
AB Phenylpurines I, phenylpteridines II, and phenylquinazolines III [R = Ph, SCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>, NHCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>, Cl, H, SMe, 4-pyridyl, S(CH<sub>2</sub>)<sub>3</sub>NMe<sub>2</sub>; R<sup>1</sup> = SCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>, Cl, NHCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>, NH<sub>2</sub>, Ph, H, SMe, S(CH<sub>2</sub>)<sub>3</sub>NMe<sub>2</sub>; R<sup>2</sup> = H, SCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>, Ph; R<sup>3</sup> = H, Me] were prepared by various routes. I (R = Ph, R<sup>1</sup> = SCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>, R<sup>2</sup> = H), II (R = Ph, R<sup>1</sup> = NHCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>, R<sup>3</sup> = Me), and III (R = Ph, R<sup>1</sup> = SCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>) have considerable activity as amplifiers of

phleomycin-G in vitro.

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S2042-, Water

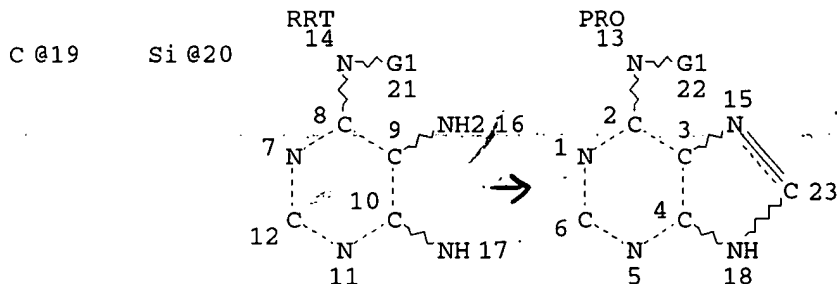


64%

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L4

STR



VAR G1=19/20

NODE ATTRIBUTES:

NSPEC    IS RC        AT    19

NSPEC    IS RC        AT    20

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS    23

STEREO ATTRIBUTES: NONE

L6                    4 SEA FILE=CASREACT SSS FUL L4 (        4 REACTIONS)

=&gt; d 16 ibib abs crd 1-4

L6    ANSWER 1 OF 4    CASREACT    COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:        106:18601    CASREACT

TITLE:                    Preparation of purine derivatives as pharmaceuticals

INVENTOR(S):             Yuki, Hiroshi; Sueoka, Hiroyuki; Yasumoto, Mitsuyoshi;  
Terasawa, Michio; Imayoshi, Tomonori

PATENT ASSIGNEE(S):     Yoshitomi Pharmaceutical Industries, Ltd., Japan

SOURCE:                  Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DOCUMENT TYPE:          Patent

LANGUAGE:                Japanese

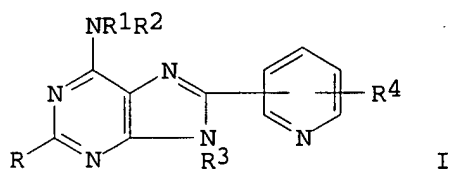
FAMILY ACC. NUM. COUNT:    1

PATENT INFORMATION:

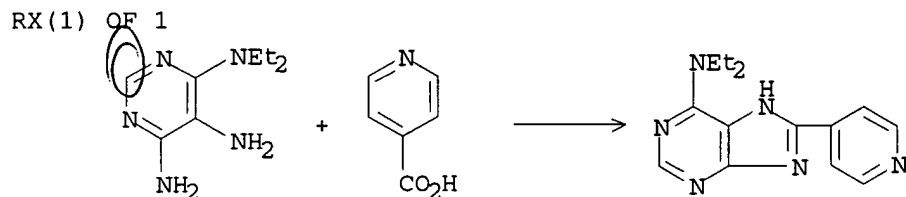
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61158983	A2	19860718	JP 1984-280057	19841228
JP 05028719	B4	19930427		
PRIORITY APPLN. INFO.:			JP 1984-280057	19841228

GI





AB The title compds. (I; R = H, Ph, substituted Ph; R1 and R2 = H, alkyl, cycloalkyl, hydroxyalkyl, etc.; R3 and R4 = H or lower alkyl) are prepared as inflammation inhibitors, analgesics, antiallergy agents, and anticoagulants (no data). Thus, 4,5-diamino-6-(diethylamino)pyrimidine was refluxed with isonicotinic acid and POCl<sub>3</sub> for 3 h to give 6-(diethylamino)-8-(4-pyridyl)purine. A tablet formulation containing I is described.



L6 ANSWER 2 OF 4 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 104:33950 CASREACT

TITLE: Purine derivatives

INVENTOR(S): Yuki, Hiroshi; Sueoka, Hiroyuki; Yasumoto, Mitsuyoshi; Terasawa, Michio; Imayoshi, Tomonori

PATENT ASSIGNEE(S): Yoshitomi Pharmaceutical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 20 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

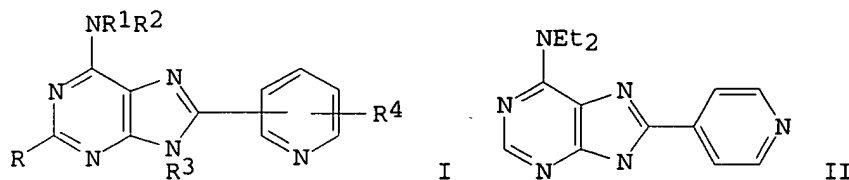
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

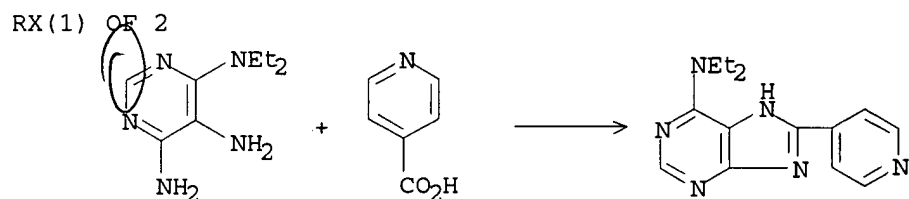
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8503077	A1	19850718	WO 1984-JP633	19841228
W: US				
RW: AT, BE, DE, FR, GB, NL, SE				
JP 60260579	A2	19851223	JP 1984-4986	19840113
EP 168500	A1	19860122	EP 1985-900502	19841228
R: AT, BE, DE, FR, GB, NL, SE				
US 4728644	A	19880301	US 1985-768535	19850722
PRIORITY APPLN. INFO.:			JP 1984-4986	19840113
			WO 1984-JP633	19841228

GI



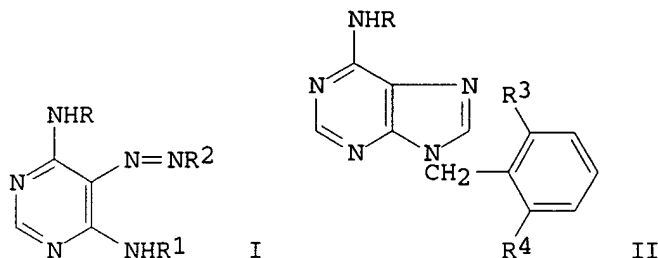
AB Title compds. I [R = H, alkyl, (un)substituted Ph; R1, R2 = H, alkyl, cycloalkyl, hydroxyalkyl, aminoalkyl, alkenyl, aralkyl; R1R2N = heterocyclic; R3, R4 = H, alkyl], useful as inflammation inhibitors, analgesics, antipyretics, antiallergics, and antithrombotics (no data), were prepared Thus, refluxing 5 g 4,5-diamino-6-diethylaminopyrimidine with 3.4 g isonicotinic acid in POCl3 for 3 h gave 3.4 g pyridylpurine II.



L6 ANSWER 3 OF 4 CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 97:162709 CASREACT  
 TITLE: Purine derivatives and intermediates  
 INVENTOR(S): Imai, Kinichi; Mano, Mitsuhiro  
 PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan  
 SOURCE: Eur. Pat. Appl., 32 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

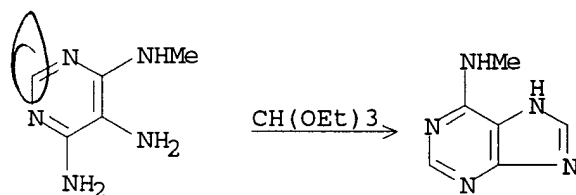
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 52959	A1	19820602	EP 1981-305192	19811030
EP 52959	B1	19860129		
R: BE, CH, DE, FR, GB, IT, NL				
JP 57085388	A2	19820528	JP 1980-161099	19801114
JP 58032867	A2	19830225	JP 1981-129518	19810818
US 4423219	A	19831227	US 1981-318277	19811104
BR 8107358	A	19820803	BR 1981-7358	19811112
DK 8105030	A	19820515	DK 1981-5030	19811113
ES 507102	A1	19830501	ES 1981-507102	19811113
HU 27622	O	19831028	HU 1981-3403	19811113
HU 187472	B	19860128		
CA 1171081	A1	19840717	CA 1981-389997	19811113
PRIORITY APPLN. INFO.:			JP 1980-161099	19801114
			JP 1981-129518	19810818

GI



AB Arylazopyrimidinediamines I (R, R1 = H, alkyl, allyl, CH2C6H3R3R4-2,6; R2 = aryl; R3,R4 = halogen) were prepared as intermediates for the coccidiostatic purines II. Thus, PhN:NCH(CN)2 was treated with HCONHMe and NH3 to give I (R = H, R1 = Me, R2 = Ph) which was reduced and cyclized with CH(OEt)3 to give 6-methylaminopurine. The latter compound was treated with 2,6-Cl(F)C6H3CH2Cl to give II (R = Me, R3 = Cl, R4 = F).

RX(7) OF 63



L6 ANSWER 4 OF 4 CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 49:23974 CASREACT  
 TITLE: Puromycin. Synthetic studies. I. Synthesis of 6-dimethylaminopurine, a hydrolytic fragment  
 AUTHOR(S): Baker, B. R.; Joseph, Joseph P.; Schaub, Robert E.  
 CORPORATE SOURCE: American Cyanamid Co., Pearl River, NY  
 SOURCE: Journal of Organic Chemistry (1954), 19, 631-7  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable

AB Alcoholysis of puromycin gives 3 cleavage products: (a) an amphoteric H2O-soluble moiety, C7H9N3 (I), (b) an aminopentose, and (c) p-MeOC6H4CH2CH(NH2)CO2Et. I has been found to be identical with 6-dimethylaminopurine (II) which is synthesized. Refluxing 33.2 g. NCCH2CO2Et and 25.6 g. SC(NH2)2 in 300 cc. absolute EtOH containing 18.4 g.

MeONa

2 hrs. with stirring, then adding 60 cc. H2O and, dropwise, 29 cc. Me2SO4, refluxing the mixture 10 min., and cooling it in ice give 82% 2-methylmercapto-4-amino-6-pyrimidinol (III), m. 261-2° (decomposition). Adding cautiously 200 cc. POCl3 to 40 g. III and 16 g. PhNMe2, refluxing the mixture 8 hrs., concentrating it in vacuo, pouring the sirup into 350 cc.

H2O,

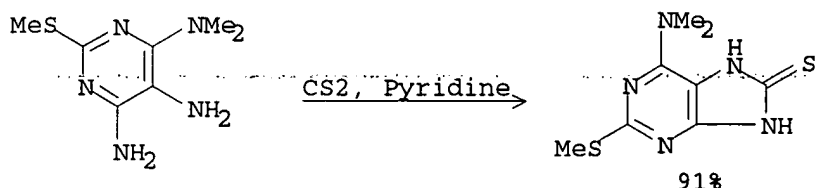
adding a slight excess of NH4OH (about 500 cc.) to the decanted solution, heating it 1 hr. on a steam bath, concentrating it to about 1/3, and

extracting the

precipitate with 25 cc. N NaOH leave 62% 2-methylmercapto-4-amino-6-chloropyrimidine (IV), m. 126-7°. Heating 12 g. IV and 30 cc. 25% aqueous Me2NH 4 hrs. in a steel bomb at 125° gives 94% 6-Me2N analog

(V), m. 162-4° [HCl derivative, 100%, m. 282° (decomposition)]. Adding in small portions 5.45 g. NaNO<sub>2</sub> in 11 cc. H<sub>2</sub>O to 11.8 g. V in 230 cc. 10% AcOH at 3° gives 94% 2-methylmercapto-4-amino-5-nitroso-6-dimethylaminopyrimidine (VI), blue crystals, m. 219-20° (decomposition). Adding (5-10 min.) in 3 portions 58 g. Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub>·2H<sub>2</sub>O to moist VI from 25 g. IV in 580 cc. H<sub>2</sub>O at 50°, adding another 20 g. Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub>·2H<sub>2</sub>O, and warming the mixture 10 min. to 70° give 89% 2-methylmercapto-4,5-diamino-6-dimethylaminopyrimidine (VII), m. 154-5°. Heating 3.4 g. VII in 34 cc. 90% HCO<sub>2</sub>H 1 hr., concentrating the solution in vacuo, dissolving the sirup in H<sub>2</sub>O, and making the solution alkaline give 85% 2-methylmercapto-4-amino-5-formamido-6-dimethylaminopyrimidine (VIII), m. 225-6° (decomposition), resolidifying at 250° and m. again 280° (decomposition). VIII is also obtained in 50% yield when Zn dust is added at 100° to 500 mg. VI in 5 cc. 90% HCO<sub>2</sub>H and the mixture is heated 0.5 hr. Refluxing 500 mg. VIII in 5 cc. HCONH<sub>2</sub> 50 min. and diluting the mixture with H<sub>2</sub>O give 330 mg. 2-methylmercapto-6-dimethylaminopurine (IX), m. 284° (slight decomposition). When VIII is boiled 10 min. with quinoline 65% IX is obtained. Heating 2.5 g. VIII 5 min. at 250° gives 99% IX and, when 2.48 g. VIII is refluxed in 30 cc. EtOH 15 min. with 10 cc. 5% NaOH and the mixture is acidified with AcOH, 70% IX is obtained. Refluxing 2 g. VII in 20 cc. C<sub>5</sub>H<sub>5</sub>N and 4 cc. CS<sub>2</sub> 0.5 hr. gives 91% 2-methylmercapto-6-dimethylamino-8-mercaptapurine (X), m. above 350°. Methylation of 1.7 g. X in 7.1 cc. N NaOMe in MeOH with 0.66 cc. Me<sub>2</sub>SO<sub>4</sub> gives 2,8-bis(methylmercapto)-6-dimethylaminopurine (XI), m. 257-9°. Similarly, 700 mg. X and PhCH<sub>2</sub>Cl in lieu of Me<sub>2</sub>SO<sub>4</sub> gives 2-methylmercapto-6-dimethylamino-8-benzylmercaptapurine, m. 230-2°. Refluxing 1 g. VIII in 100 cc. EtOH with 1.33 teaspoonfuls of desulfurizing Raney Ni 0.5 hr. gives 69% 4-amino-5-formamido-6-dimethylaminopyrimidine (XII), m. 185-7° (decomposition). Heating 500 mg. IX in 40 cc. N NaOH, adding 3 cc. Raney Ni to the clear solution, heating the mixture 0.5 hr. on a steam bath, evaporating the filtered and acidified (AcOH) solution in vacuo, dissolving the residue in 10 cc. H<sub>2</sub>O, extracting with ether, and evaporating the dried ether extract give 43% II, m. 257-8°, which gives no m.p. depression when mixed with I [picrate of II, m. 244-5° (decomposition)]. II is also obtained in 16% yield when 600 mg. XI is heated 0.5 hr. in 60 cc. MeOCH<sub>2</sub>CH<sub>2</sub>OH, in 17% yield when 800 mg. IX heated 0.5 hr. in 80 cc. MeOCH<sub>2</sub>CH<sub>2</sub>OH and 3.3 cc. N NaOMe in MeOH with 2.67 teaspoonfuls of Raney Ni, in 83% yield when 200 mg. XII is refluxed 10 min. in 2 cc. quinoline, or in 85% yield on fusion of 100 mg. XII at 250-5°. The ultraviolet and infrared absorption spectra of II from I and the synthetic II are identical.

RX(1) OF 3



NOTE: Classification: Heterocycle formation; Condensation; Isomerisation; # Conditions: pyridine 30mn st bath



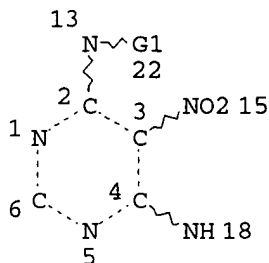
=> d que

L8

STR

C @19

Si @20



*Reactant*

VAR G1=19/20

NODE ATTRIBUTES:

NSPEC IS RC AT 19

NSPEC IS RC AT 20

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

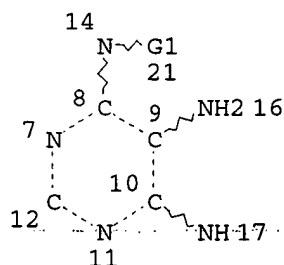
STEREO ATTRIBUTES: NONE

L10 1849 SEA FILE=REGISTRY SSS FUL L8

L11 STR

C @19

Si @20



*Reactant*

*Product*

VAR G1=19/20

NODE ATTRIBUTES:

NSPEC IS RC AT 19

NSPEC IS RC AT 20

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

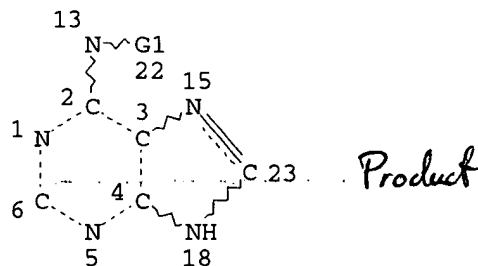
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L13 293 SEA FILE=REGISTRY SSS FUL L11

L14 STR

C @19    si @20



VAR G1=19/20

NODE ATTRIBUTES:

NSPEC    IS RC        AT    19

NSPEC    IS RC        AT    20

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS    13

STEREO ATTRIBUTES: NONE

L16            3658 SEA FILE=REGISTRY SSS FUL L14

L17            91 SEA FILE=HCAPLUS ABB=ON    PLU=ON    L10(L) (RACT OR RCT OR RGT)/RL

L18            92 SEA FILE=HCAPLUS ABB=ON    PLU=ON    L13(L) PREP/RL

L19            34 SEA FILE=HCAPLUS ABB=ON    PLU=ON    L17 AND L18

L20            863 SEA FILE=HCAPLUS ABB=ON    PLU=ON    L16(L) PREP/RL

L21            47 SEA FILE=HCAPLUS ABB=ON    PLU=ON    L13(L) (RACT OR RCT OR RGT)/RL

L22            9 SEA FILE=HCAPLUS ABB=ON    PLU=ON    L20 AND L21

L23            1 SEA FILE=HCAPLUS ABB=ON    PLU=ON    L19 AND L22

=&gt; d l23 ibib abs hitind hitstr

L23    ANSWER 1 OF 1    HCAPLUS    COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:        1987:84257    HCAPLUS

DOCUMENT NUMBER:        106:84257

TITLE:                    Heterocyclic amplifiers of phleomycin. VI. Some phenylpurines, phenylpteridines, phenylquinazolines and related compounds

AUTHOR(S):                Brown, Desmond J.; Mori, Kenya

CORPORATE SOURCE:        John Curtin Sch. Med. Res., Aust. Natl. Univ., Canberra, 2601, Australia

SOURCE:                    Australian Journal of Chemistry (1985), 38(3), 467-74

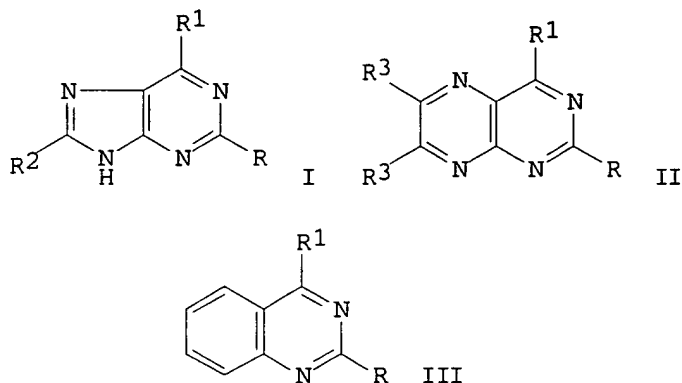
CODEN: AJCHAS; ISSN: 0004-9425

DOCUMENT TYPE:            Journal

LANGUAGE:                 English

OTHER SOURCE(S):         CASREACT 106:84257

GI



AB Phenylpurines I, phenylpteridines II, and phenylquinazolines III [R = Ph, SCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>, NHCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>, Cl, H, SMe, 4-pyridyl, S(CH<sub>2</sub>)<sub>3</sub>NMe<sub>2</sub>; R<sup>1</sup> = SCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>, Cl, NHCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>, NH<sub>2</sub>, Ph, H, SMe, S(CH<sub>2</sub>)<sub>3</sub>NMe<sub>2</sub>; R<sub>2</sub> = H, SCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>, Ph; R<sub>3</sub> = H, Me] were prepared by various routes. I (R = Ph, R<sup>1</sup> = SCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>, R<sub>2</sub> = H), II (R = Ph, R<sup>1</sup> = NHCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>, R<sub>3</sub> = Me), and III (R = Ph, R<sup>1</sup> = SCH<sub>2</sub>CH<sub>2</sub>NMe<sub>2</sub>) have considerable activity as amplifiers of phleomycin-G in vitro.

CC 26-9 (Biomolecules and Their Synthetic Analogs)

Section cross-reference(s): 10

IT 34375-69-4P 58549-90-9P 106823-66-9P **106823-68-1P**  
 106823-69-2P 106823-70-5P 106823-71-6P 106823-77-2P 106823-78-3P  
 106823-81-8P 106823-82-9P 106823-83-0P 106823-85-2P 106823-94-3P  
 106823-95-4P 106823-99-8P 106824-00-4P 106824-01-5P 106824-02-6P

RL: SPN (Synthetic preparation); **PREP (Preparation)**  
 (preparation and phleomycin amplifying activity of)

IT **106823-76-1P**

RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**  
 (preparation and reaction of, with glyoxal)

IT **106823-75-0P** 106823-90-9P

RL: ~~RCT (Reactant)~~; ~~SPN (Synthetic preparation)~~; ~~PREP (Preparation)~~; **RACT (Reactant or reagent)**  
 (preparation and reduction of)

IT 18602-79-4P 50680-79-0P 106823-84-1P 106823-86-3P 106823-87-4P  
 106823-88-5P 106823-89-6P 106823-98-7P **106824-03-7P**  
 107667-61-8P

RL: SPN (Synthetic preparation); **PREP (Preparation)**  
 (preparation of)

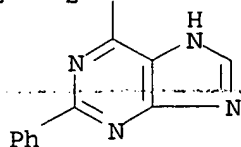
IT **106823-68-1P**

RL: SPN (Synthetic preparation); **PREP (Preparation)**  
 (preparation and phleomycin amplifying activity of)

RN 106823-68-1 HCAPLUS

CN 1,2-Ethanediamine, N,N-dimethyl-N'-(2-phenyl-1H-purin-6-yl)- (9CI) (CA  
 INDEX NAME)

Me<sub>2</sub>N-CH<sub>2</sub>-CH<sub>2</sub>-NH



*Product*

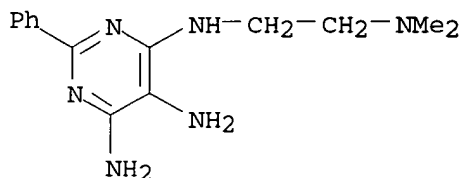


IT 106823-76-1P

RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
 (Preparation); **RACT** (Reactant or reagent)  
 (preparation and reaction of, with glyoxal)

RN 106823-76-1 HCAPLUS

CN 4,5,6-Pyrimidinetriamine, N4-[2-(dimethylamino)ethyl]-2-phenyl- (9CI) (CA  
 INDEX NAME).



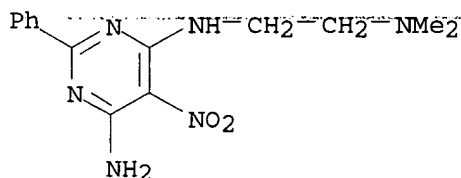
Reactant  
 +  
 Product } Intermediate?

IT 106823-75-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation and reduction of)

RN 106823-75-0 HCAPLUS

CN 4,6-Pyrimidinediamine, N-[2-(dimethylamino)ethyl]-5-nitro-2-phenyl- (9CI)  
 (CA INDEX NAME)



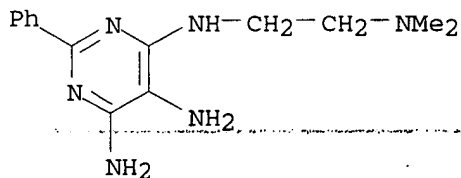
Reactant

IT 106824-03-7P

RL: SPN (Synthetic preparation); **PREP** (Preparation)  
 (preparation of)

RN 106824-03-7 HCAPLUS

CN 4,5,6-Pyrimidinetriamine, N4-[2-(dimethylamino)ethyl]-2-phenyl-,  
 dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl